Naval Nuclear Laboratory
Special Purpose O-17, O-18, Be-9 (α,n) Evaluations

Jesse Holmes
Andrew Pavlou
Jason Thompson
Mike Zerkle

Cross Section Evaluation Working Group

Brookhaven National Laboratory

November 5-7, 2018

The Naval Nuclear Laboratory is operated for the U.S. Department of Energy by
Fluor Marine Propulsion (FMP), LLC, a wholly owned subsidiary of Fluor Corporation.

NAVAL NUCLEAR LABORATORY

Applications for Special Purpose (α,n) Libraries

- Calculation of yield and spectrum of neutrons produced by (α,n) reactions with light nuclides in materials containing actinide α-particle emitters.
- Non-fission neutron source characterization for reactor analysis, Am-Be / Pu-Be sources and shielding, nuclear safeguards, materials non-destructive assay, etc.
- JENDL/AN-2005 includes ENDF-6 format (α,n) evaluations for 17 nuclides with $Z \leq 14$. No (α,n) evaluations are available in ENDF/B.
- The LANL code SOURCES is considered an industry standard for (α,n) neutron source characterization.
- NNL recently implemented an in-line (α,n) source sampling methodology in MC21 for Monte Carlo radiation transport simulations. The LLNL Monte Carlo code COG uses a similar approach, but only the ability to calculate neutron yields has been studied.
- Other Monte Carlo codes exist that use various methods enabling (α,n) calculations (MCNP, FLUKA, GEANT, SRIM/TRIM, etc.) but suffer from a variety of disadvantages (transport expense, manual input requirements, geometry limitations, etc.).

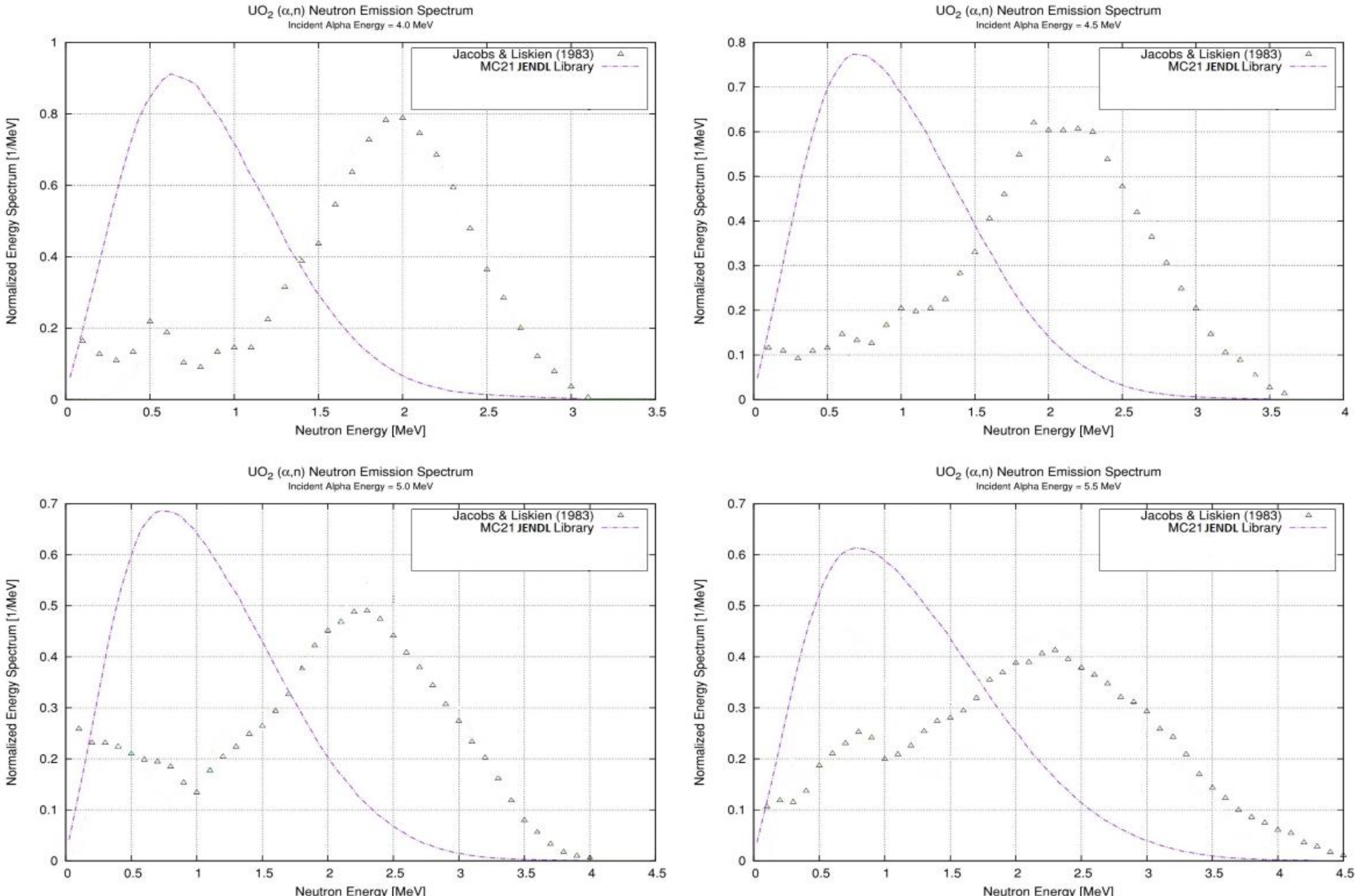
NAVAL NUCLEAR LABORATORY

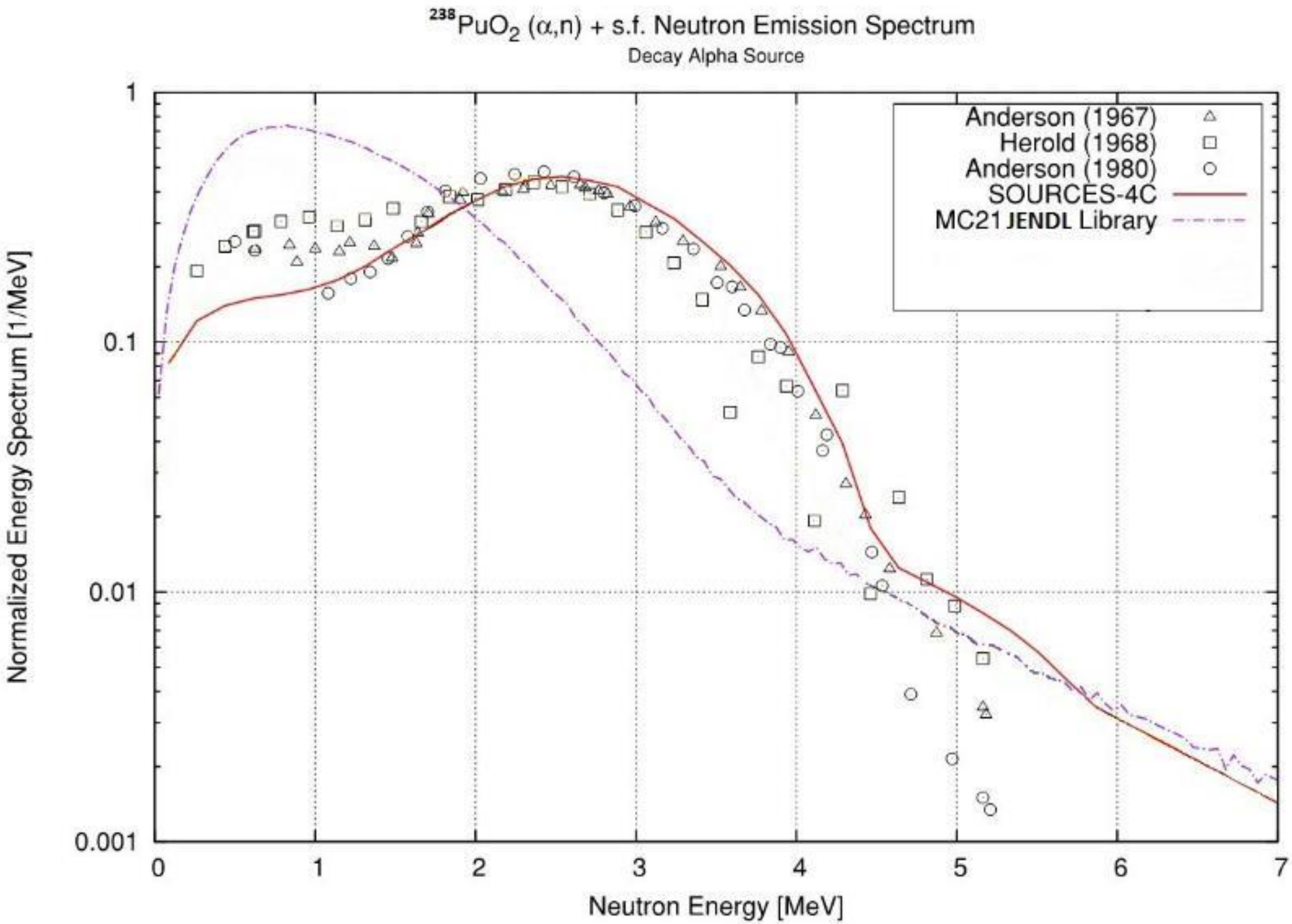
Testing JENDL/AN-2005 (α,n) Evaluations

- NNL tested the JENDL/AN-2005 (α,n) evaluations in MC21.
- Calculated neutron yields and energy/angle spectra were compared to available experimentally measured data from public literature.
- MC21 neutron yield results compared very well with most experimental data.
- For neutron energy spectra, MC21 results were noted to deviate significantly from published experimental data for $^{natural}UO_2$, $^{238}PuO_2$, and Am-Be sources.
- The deviations were determined to be caused by physics deficiencies in the JENDL/AN-2005 evaluations for O-17, O-18, and Be-9.
- NNL modified these evaluations to address the identified deficiencies and validated the new versions against experimental data.
- NNL is now submitting these modified special-purpose (α,n) evaluations for inclusion in ENDF/B-VIII.1.

NAVAL NUCLEAR LABORATORY

Natural-Uranium UO_2 (α,n) Neutron Spectra
JENDL Library Testing for O-17,18





NAVAL NUCLEAR LABORATORY

Problems with Kalbach-Mann Systematics

- O-17 and O-18 use Kalbach-Mann systematics for File 6 coupled energy/angle distributions for MT=4 (production of one neutron in the exit channel).

- Energy/angle distributions based on Kalbach-Mann systematics are decoupled from the partial cross sections for reactions leaving the residual in the ground state or particular low-level excited states.

- The Q-values of low-level n^{th} excited-state reactions (including the 0^{th} ground-state) are widely separated and strongly impact the emitted neutron energy spectrum for reactions induced by low-energy α particles.

- Kalbach-Mann theory for (α,n) neutron energy/angle distributions is appropriate for very-high-energy incident α particles (tens to hundreds of MeV), where high-level residual excited states (or a continuum excited state) dominate.
  - Not appropriate for low-energy α particles emitted by actinide decay (approx. 4-7 MeV), which will then undergo slowing down in materials of interest.

NAVAL NUCLEAR LABORATORY

File 6 Neutron Energy/Angle Modifications for O-17,18

(File 3 cross sections are unchanged)

MT	Reaction	Description
4	(α,n)	Production of one neutron in the exit channel. Sum of MT=50-91.
16	(α,2n)	Production of two neutrons and a residual.
22	(α,nα')	Production of a neutron and an α particle, plus a residual.
28	(α,np)	Production of a neutron and a proton, plus a residual.
50-90	(α,n_{0-40})	Production of a neutron, with the residual in the 0^{th}-40^{th} excited state.
91	(α,n_c)	Production of a neutron in the continuum not included in the above discrete representation.
201	(α,Xn)	Total neutron production.

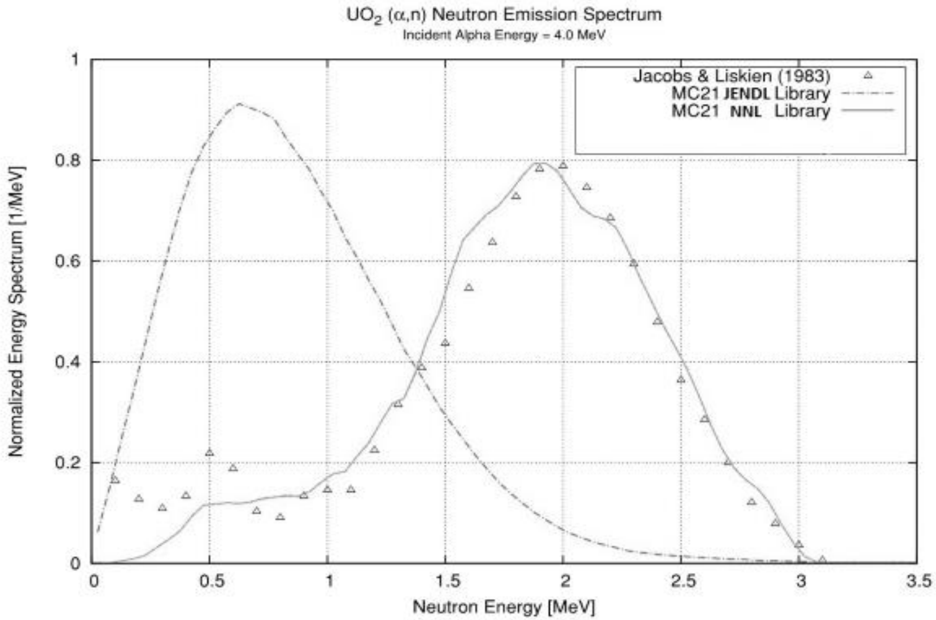
Nuclide	Cross Section MF3 MTs	JENDL version MF6 MTs	NNL version MF6 MTs
O17	4 22 50-53 91 201	4 22	22 50-53 91
O18	4 16 22 50-54 91 201	4 16 22	16 22 50-54 91

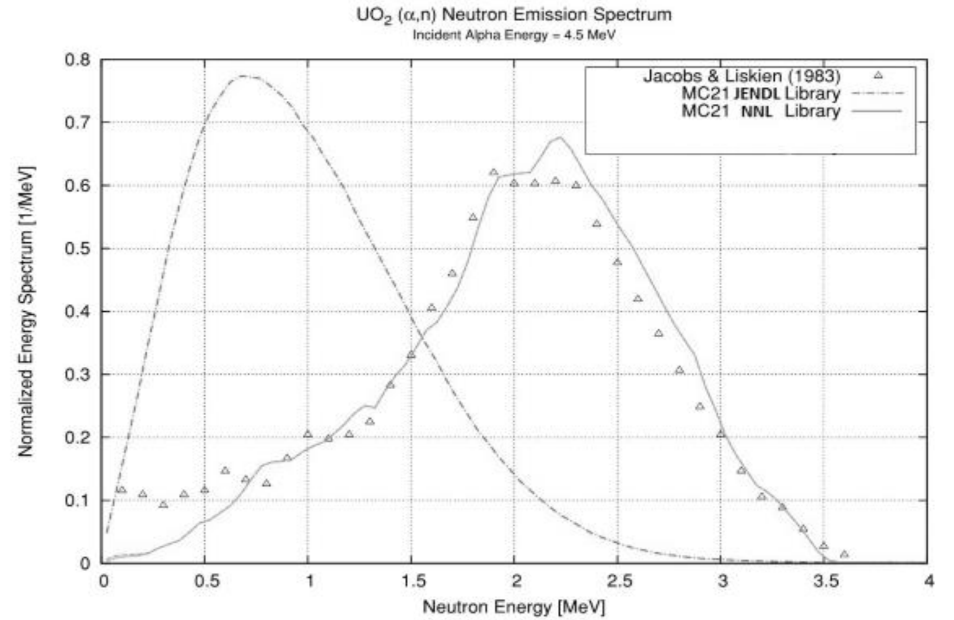
Color-coded MT values indicate neutron energy/angle distribution treatment

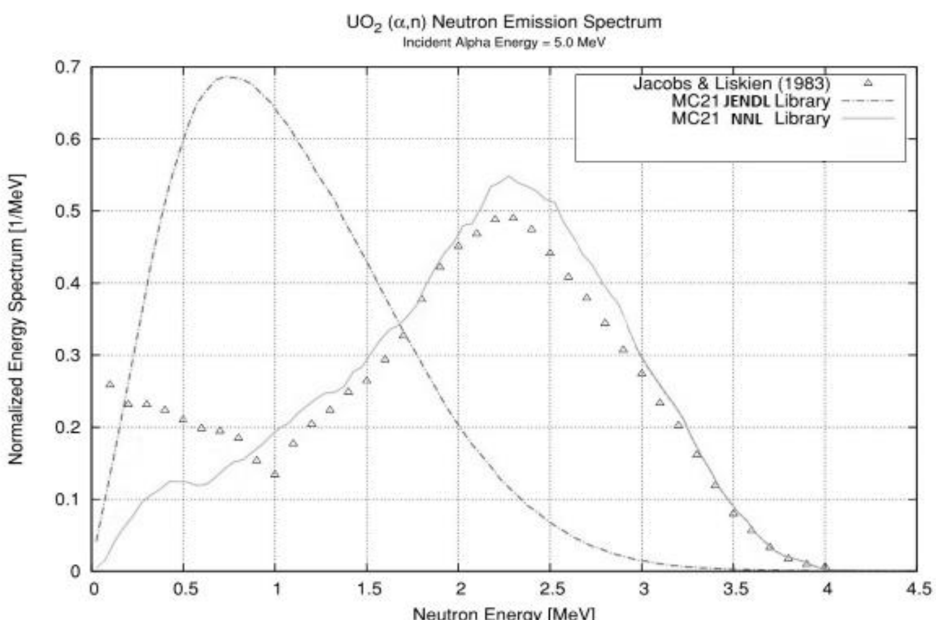
Green: Kalbach-Mann coupled energy/angle distribution
Red: Isotropic two-body kinematics

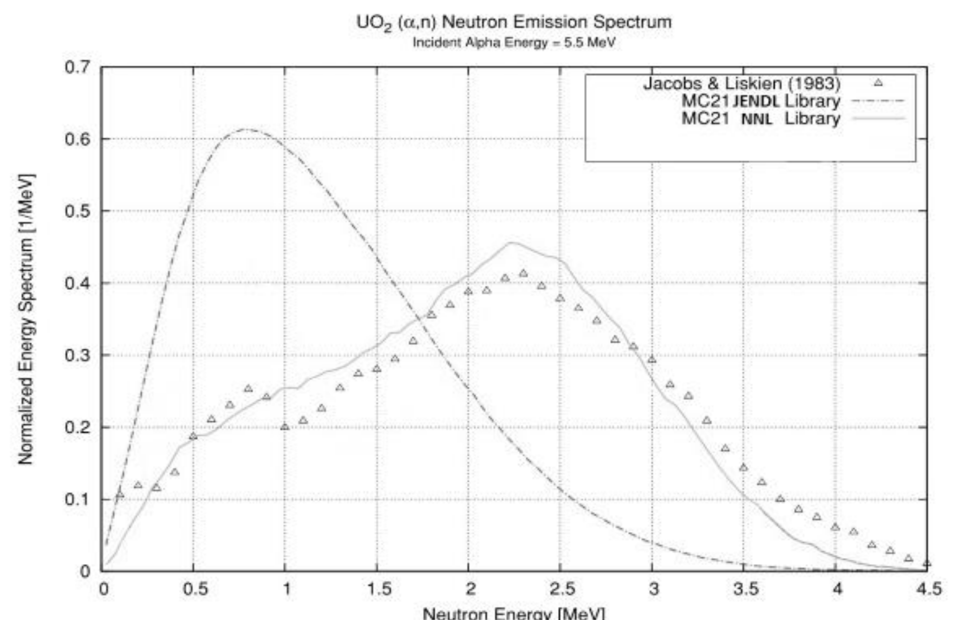
NAVAL NUCLEAR LABORATORY

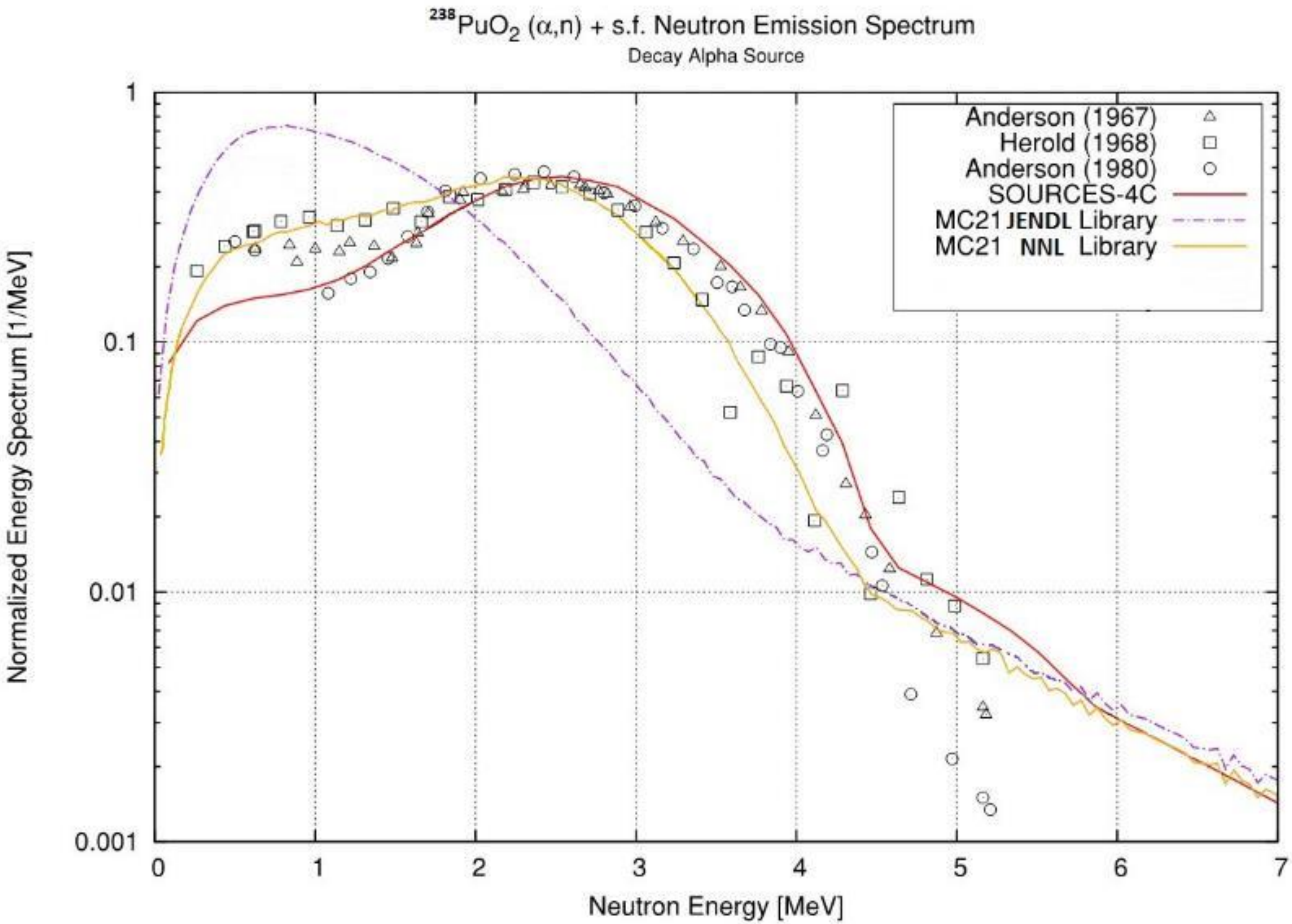
Natural-Uranium UO_2 (α,n) Neutron Spectra
JENDL vs. NNL Library Performance for O-17,18



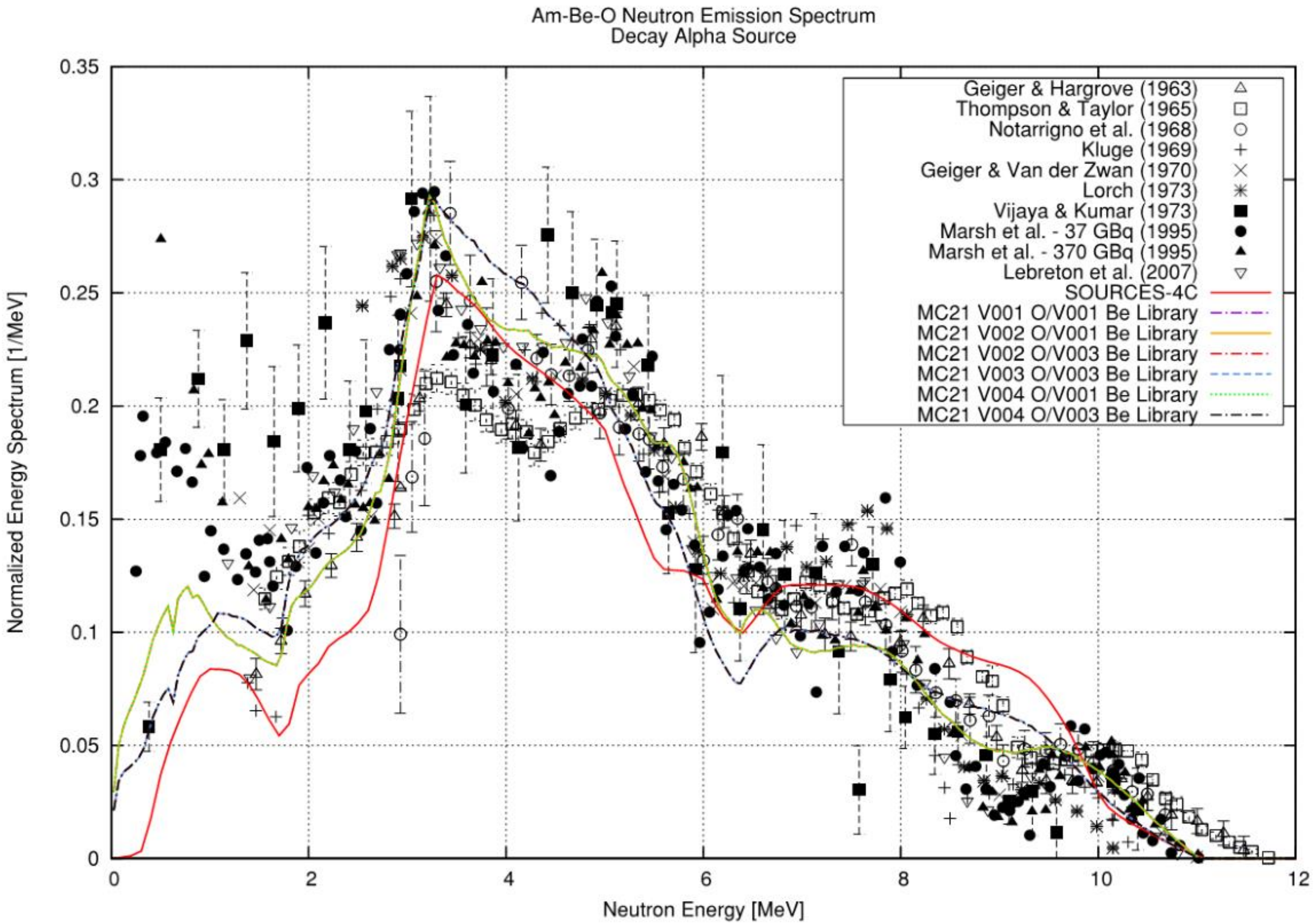








NAVAL NUCLEAR LABORATORY



NAVAL NUCLEAR LABORATORY

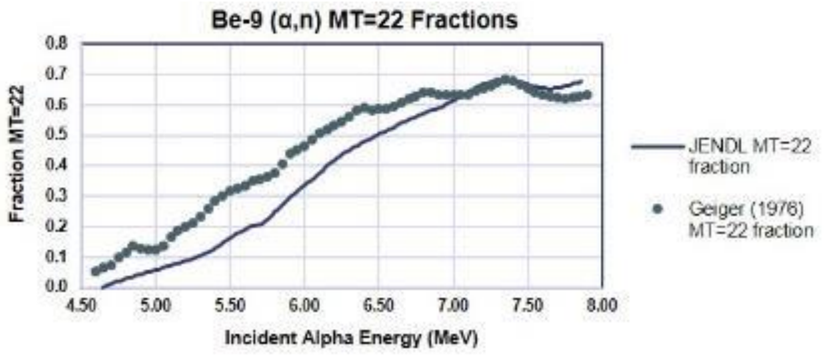
Be-9 Breakup Reaction

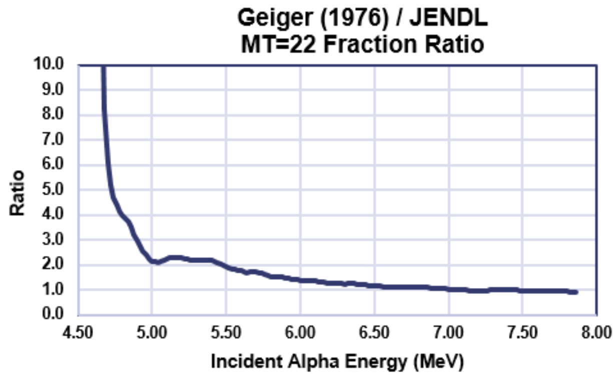
$^9Be(\alpha,\alpha')^9Be^* \rightarrow {}^8Be+n$ (included in MT=22)

JENDL uses Gibbons (1965) to fit MT=201 total XSs. Then, MT=22 is calculated based on Obst (1972).

Van der Zwan and Geiger (1970) is used for MT=50-52,91 ratios, but not for normalization.

MT=4 (MT=50-52+91) is calculated by **subtracting** MT=22 from MT=201.

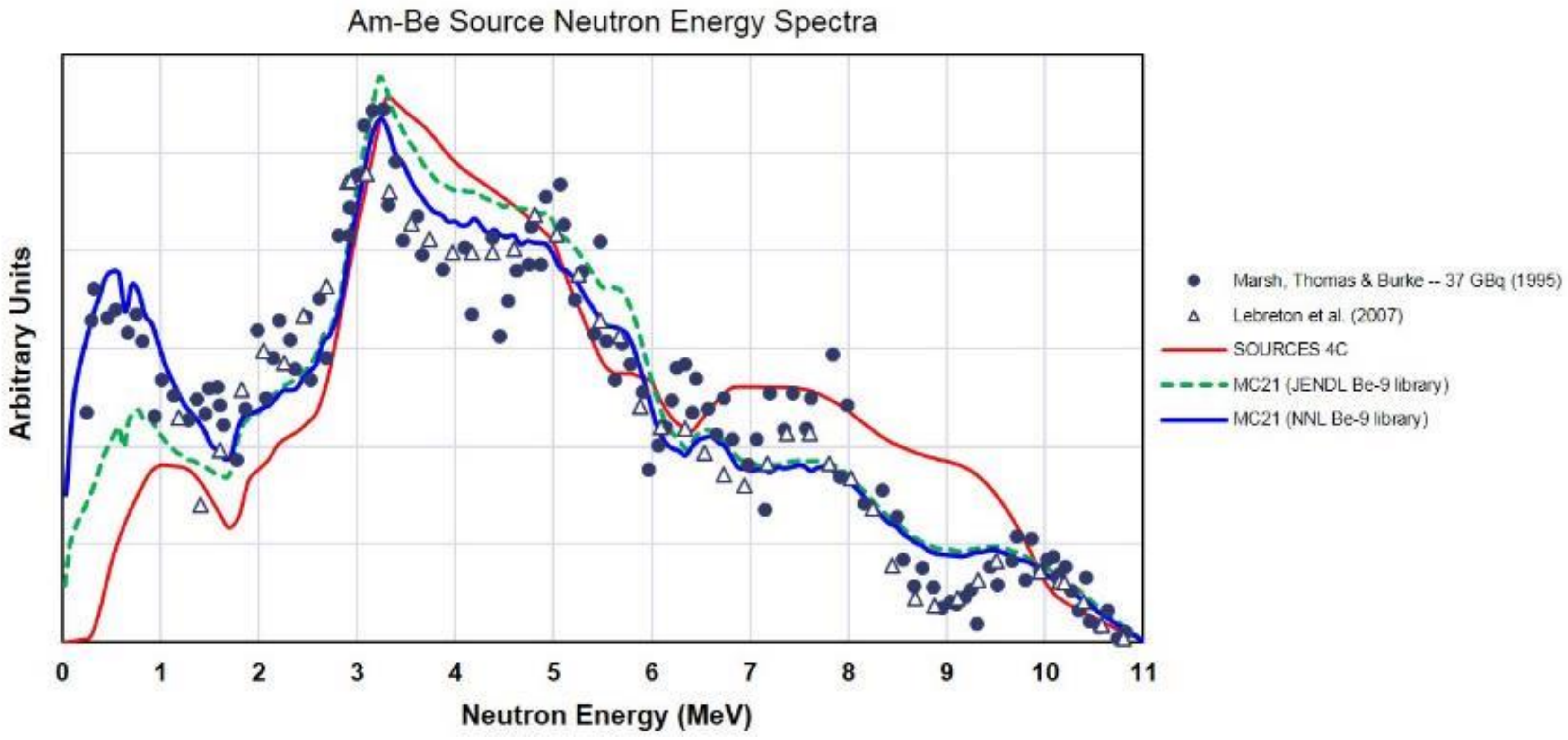




NAVAL NUCLEAR LABORATORY

Be-9 File 3 Cross Section Modifications and Am-Be Results

JENDL MT=201 (MT=4 + MT=22) data was not modified. MT=22 cross sections were modified to be consistent with the MT=22 / MT=201 ratios experimentally measured by Geiger (1975). MT=4 (MT=50-52 + MT=91) cross sections were modified to maintain consistency with MT=201. MT=50-52,91 were rescaled to maintain consistency with MT=4 changes.



NAVAL NUCLEAR LABORATORY

Summary

- NNL-modified special-purpose (α,n) evaluations for O-17, O-18, and Be-9 are being submitted for inclusion in ENDF/B-VIII.1.

- These evaluations are based on the original JENDL/AN-2005 evaluations with specific modifications by NNL to address physics deficiencies affecting neutron energy spectra. The NNL versions have been validated against experimental measurements.

- Other JENDL/AN-2005 (α,n) evaluations were tested by NNL. These are not being submitted by NNL as no modifications were made.

- For O-17, MF=3 cross sections are unchanged. MF=6 / MT=4 (using Kalbach-Mann) is removed and replaced with MF=6 / MT=50-53 (using isotropic two-body kinematics) and MF=6 / MT=91 (using original MF=6 / MT=4 Kalbach-Mann distribution). MF=6 / MT=22 is unchanged.

- For O-18, MF=3 cross sections are unchanged. MF=6 / MT=4 (using Kalbach-Mann) is removed and replaced with MF=6 / MT=50-54 (using isotropic two-body kinematics) and MF=6 / MT=91 (using original MF=6 / MT=4 Kalbach-Mann distribution). MF=6 / MT=16,22 are unchanged.

- For Be-9, MF=3 / MT=4,22 are modified to give ratios consistent with Geiger (1975). MF=3 / MT=201 is unchanged. MF=3 / MT=50-52,91 ratios are unchanged, but values are rescaled to be consistent with modifications to MF=3 / MT=4. MF=6 distributions are unchanged.

NAVAL NUCLEAR LABORATORY